Supporting Information
(14 pages including this)

Chemisorption of Hydrogen Atoms on the Sidewalls of Armchair Single-Walled Carbon Nanotubes

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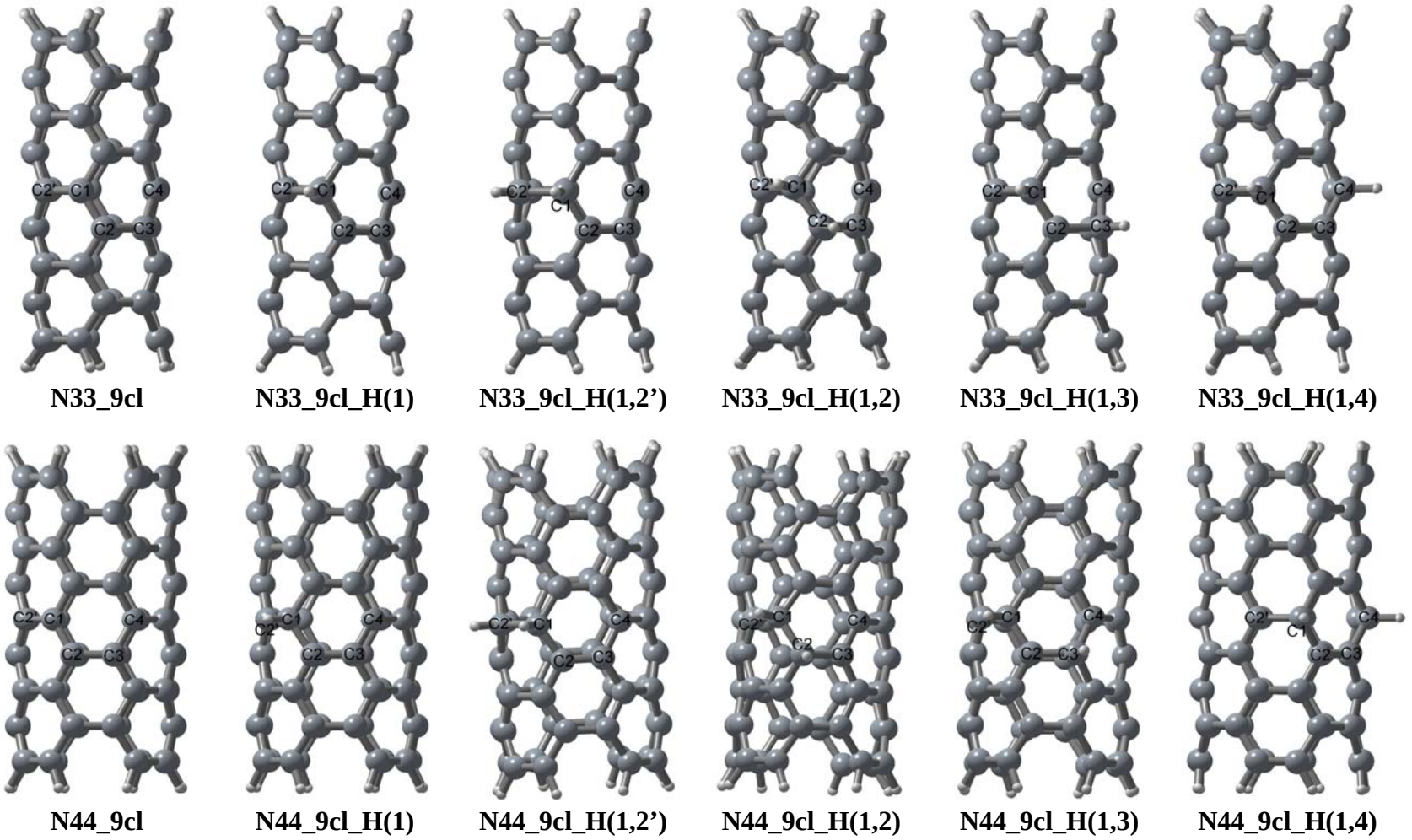
Table S1. The total energies (in Hartrees) obtained at the B3LYP/6-31G(d) level for the hydrogen chemisorbed and pristine (3,3), (4,4), (5,5) and (6,6) SWNTs.

9 carbon layers		15 carbon layers	
		(3,3) SWNT	
NT33_9cl	-2064.47082	**NT33_15cl**	-3436.00158
H(1)	-2065.05631	**H(1)**	-3436.60104
H(1,2')	-2065.67828	**H(1,2')**	-3437.2372
H(1,2)	-2065.68075	**H(1,2)**	-3437.22417
H(1,3)	-2065.62047	**H(1,3)**	-3437.16449
H(1,4)	-2065.65312	**H(1,4)**	-3437.21386
H(1,2')a	-2065.71650	**H(1,2')a**	-3437.22208
		H(1,2')b	-3437.20594
		(4,4) SWNT	
NT44_9cl	-2753.14759	**NT44_15cl**	-4582.29374
H(1)	-2753.73075	**H(1)**	-4582.87018
H(1,2')	-2754.33259	**H(1,2')**	-4583.47260
H(1,2)	-2754.31905	**H(1,2)**	-4583.46784
H(1,3)	-2754.27289	**H(1,3)**	-4583.41613
H(1,4)	-2754.33176	**H(1,4)**	-4583.46298
		(5,5) SWNT	
NT55_9cl	-3441.75412	**NT55_15cl**	-5728.41615
H(1)	-3442.32929	**H(1)**	-5728.99188
H(1,2')	-3442.91405	**H(1,2')**	-5729.57991
H(1,2)	-3442.92886	**H(1,2)**	-5729.58470
H(1,3)	-3442.86408	**H(1,3)**	-5729.52950
H(1,4)	-3442.92995	**H(1,4)**	-5729.58345
		(6,6) SWNT	
NT66_9cl	-4130.32537	**NT66_15cl**	-6874.46377
H(1)	-4130.88747	**H(1)**	-6875.03541
H(1,2')	-4131.46003	**H(1,2')**	-6875.61715
H(1,2)	-4131.48620	**H(1,2)**	-6875.62955
H(1,3)	-4131.41832	**H(1,3)**	-6875.56962
H(1,4)	-4131.48768	**H(1,4)**	-6875.62986



N33_9cl **N33_9cl_H(1)** **N33_9cl_H(1,2')** **N33_9cl_H(1,2)** **N33_9cl_H(1,3)** **N33_9cl_H(1,4)**

N44_9cl **N44_9cl_H(1)** **N44_9cl_H(1,2')** **N44_9cl_H(1,2)** **N44_9cl_H(1,3)** **N44_9cl_H(1,4)**

Figure S1 (contd.)

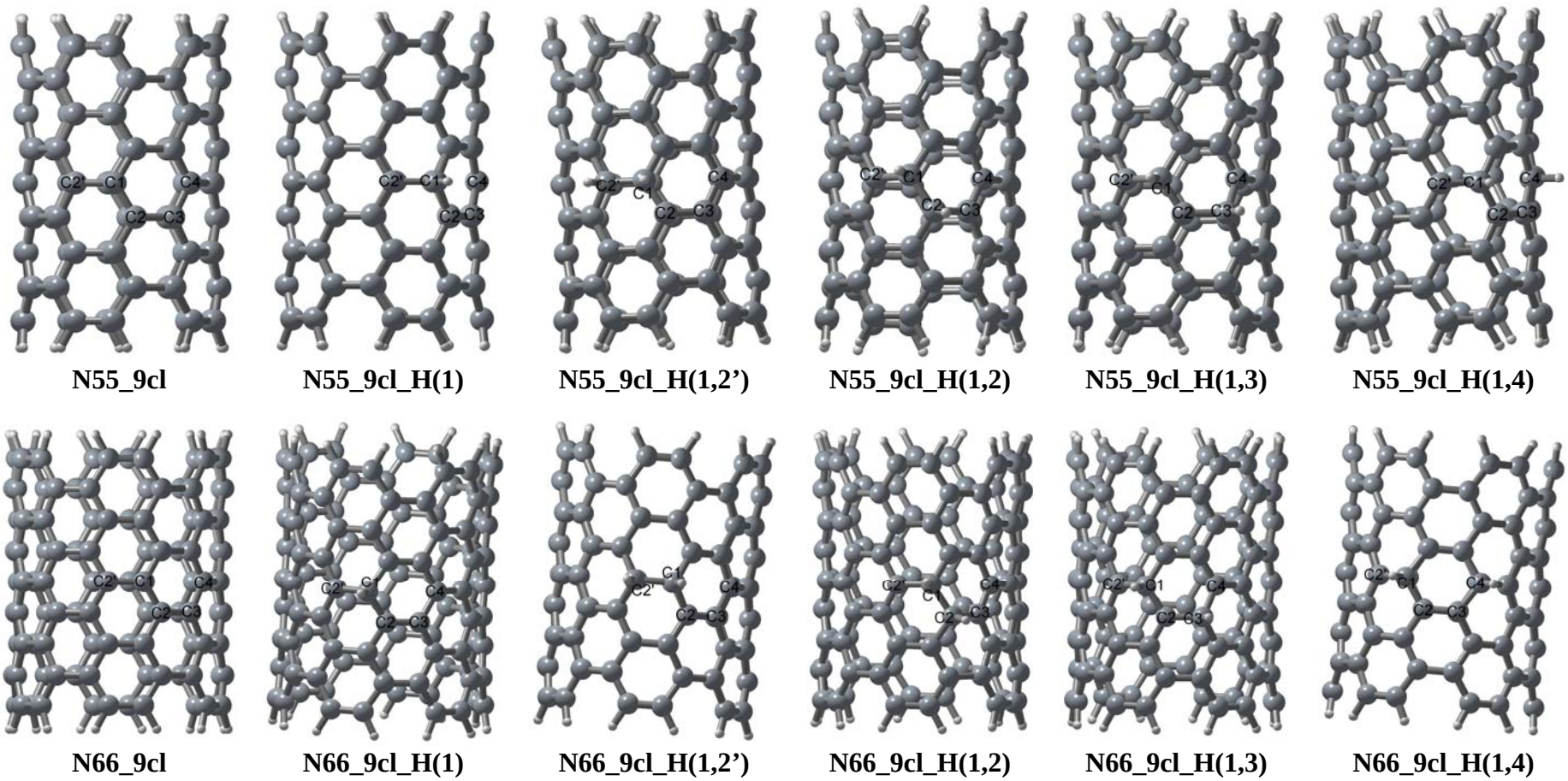
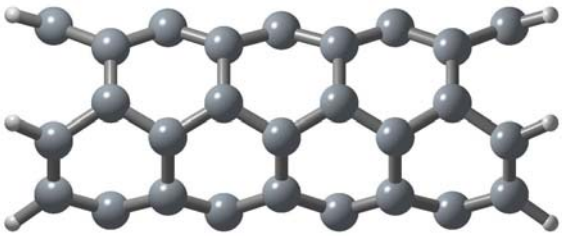
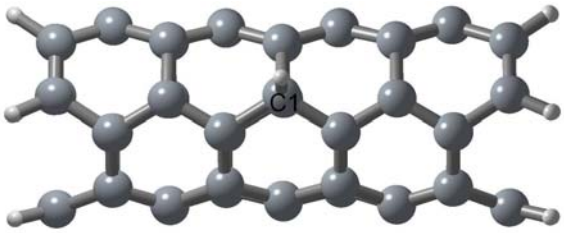


Figure S1: B3LYP/6-31G(d) optimized geometries of 9 carbon layered nanotubes of (3,3), (4,4), (5,5) and (6,6) armchair SWNTs and their one and two hydrogen chemisorbed structures in vertical view.



N33_9cl



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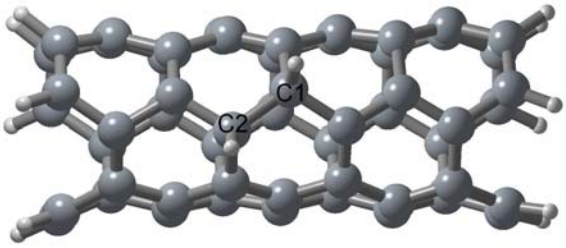

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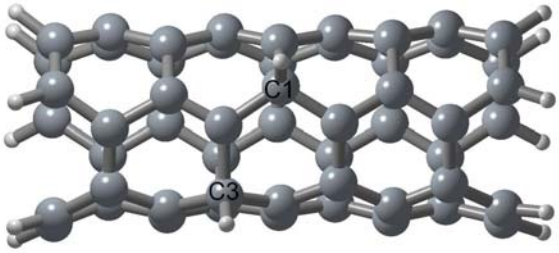

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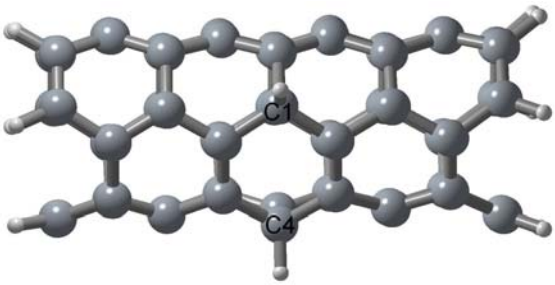

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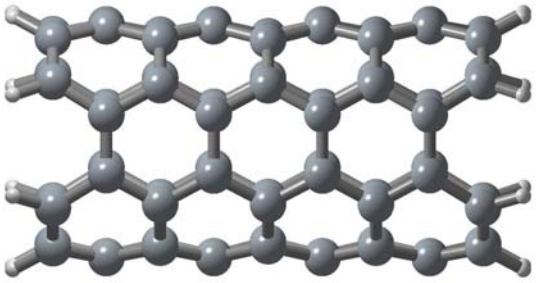

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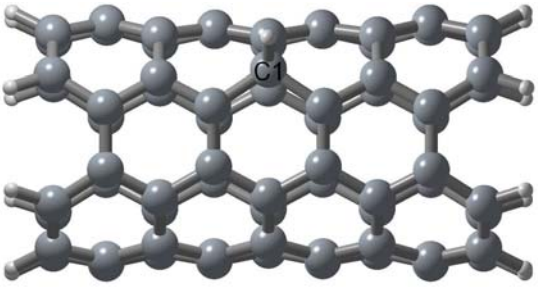

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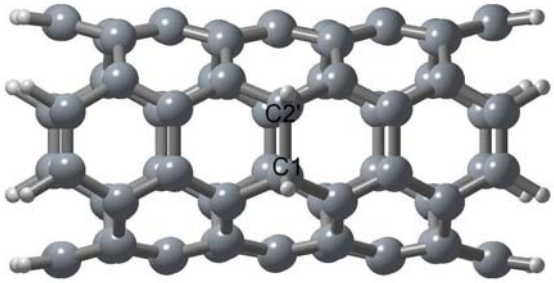

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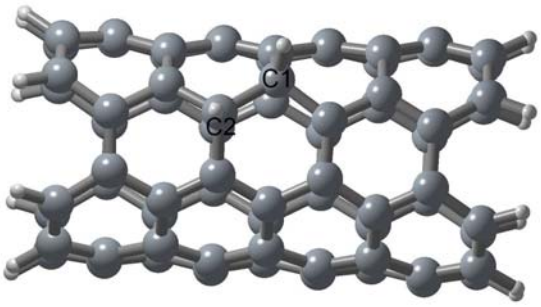

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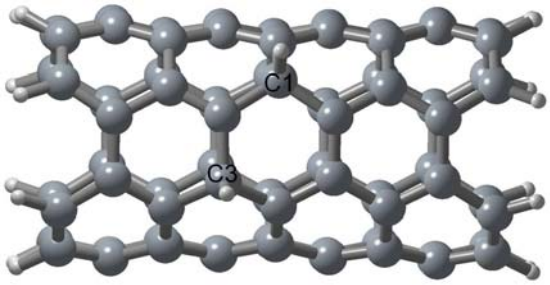

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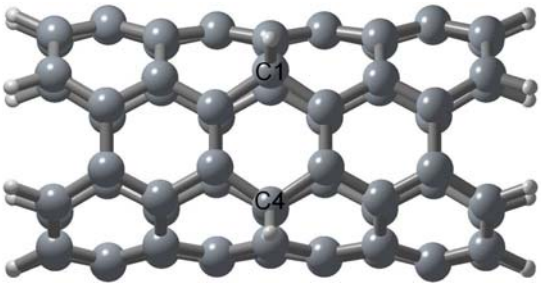

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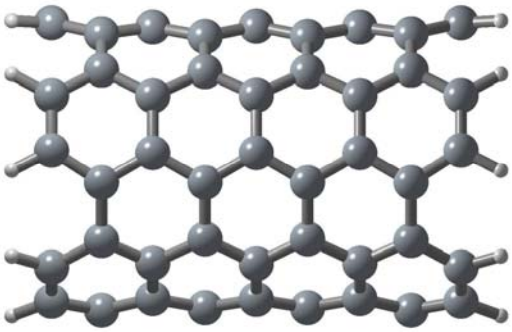

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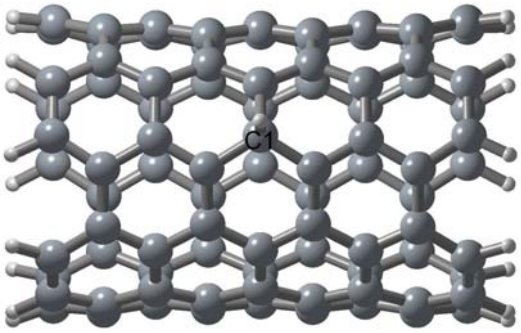

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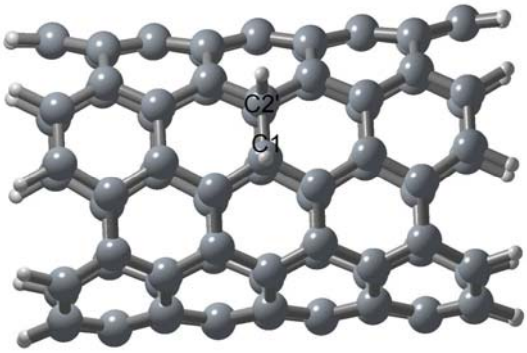

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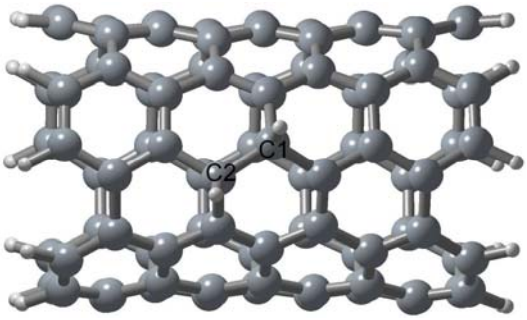

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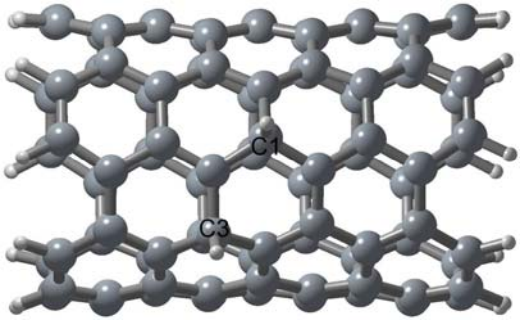

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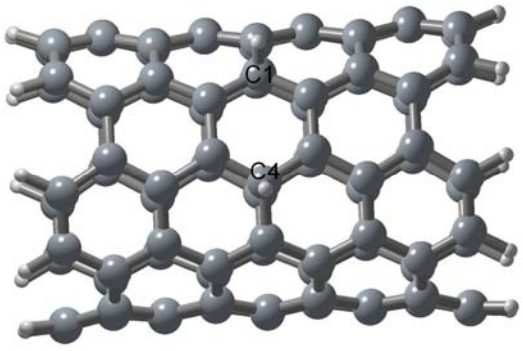

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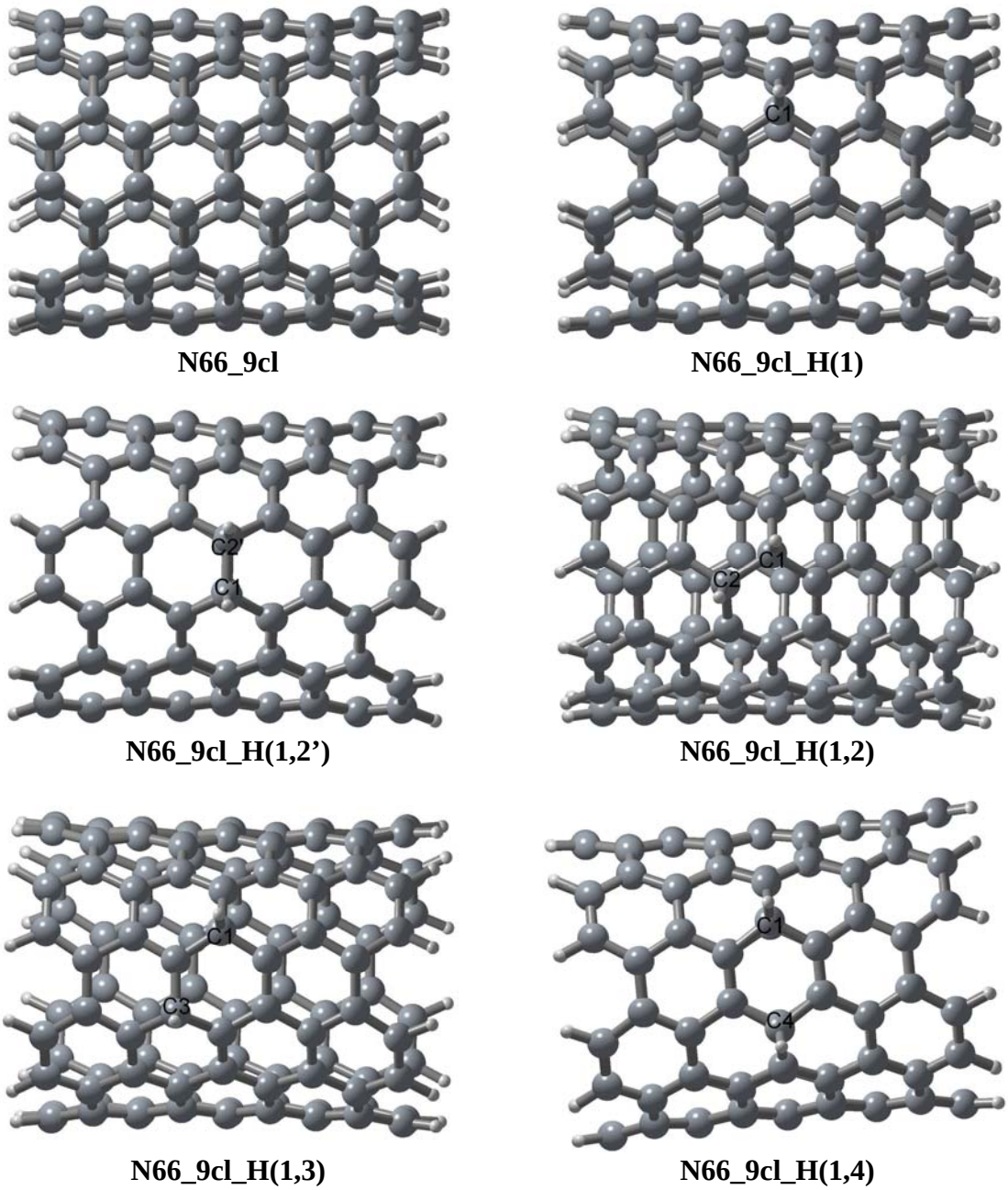
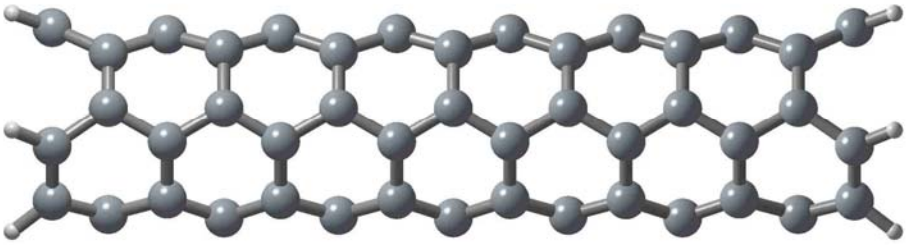
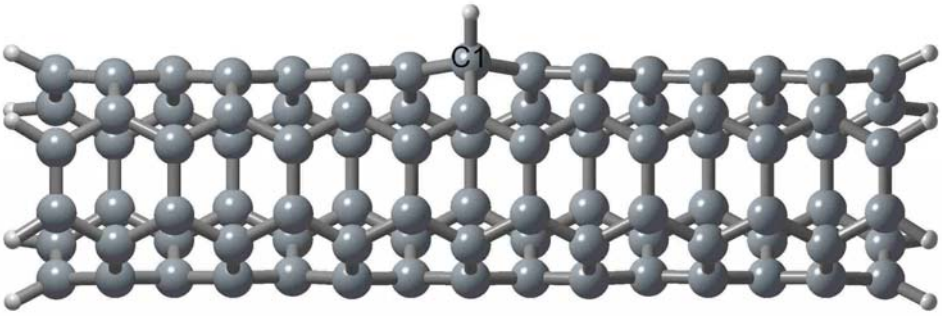


Figure S2: B3LYP/6-31G(d) optimized geometries of 9 carbon layered nanotubes of (3,3), (4,4), (5,5) and (6,6) armchair SWNTs and their one and two hydrogen chemisorbed structures in horizontal view.



N33_15cl



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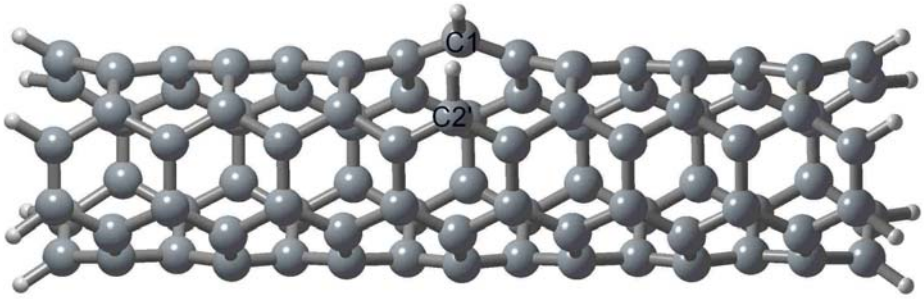

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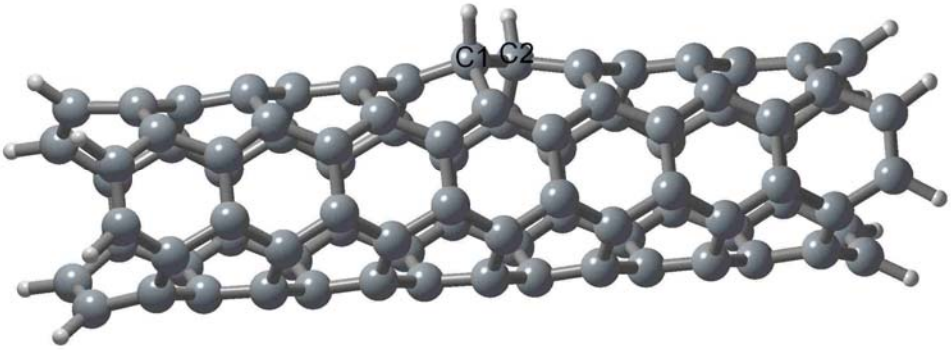

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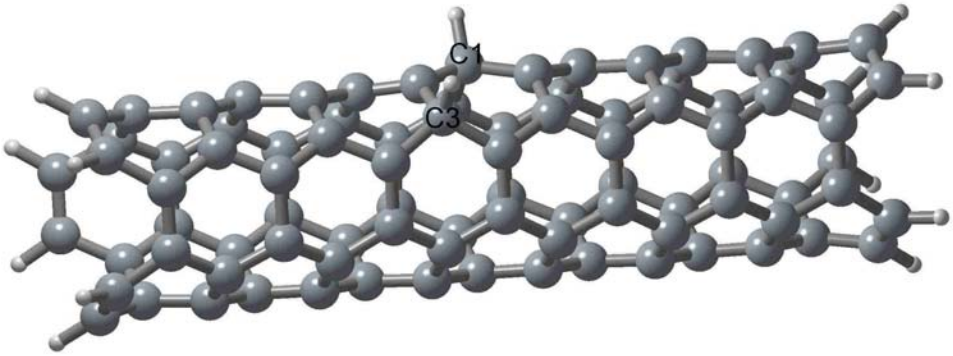

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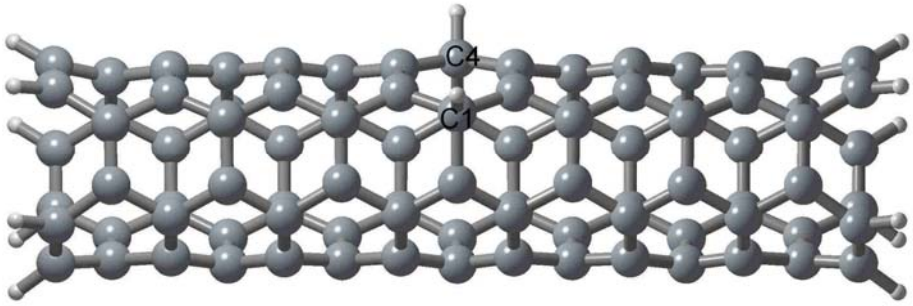

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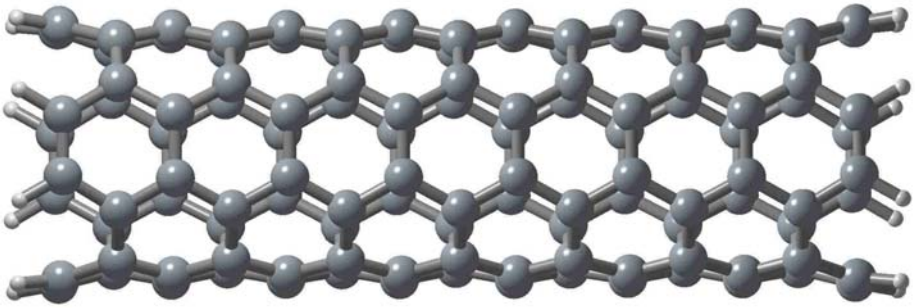

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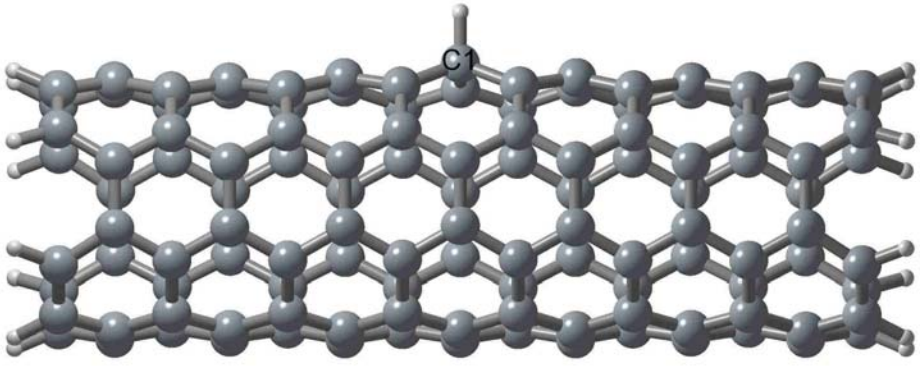

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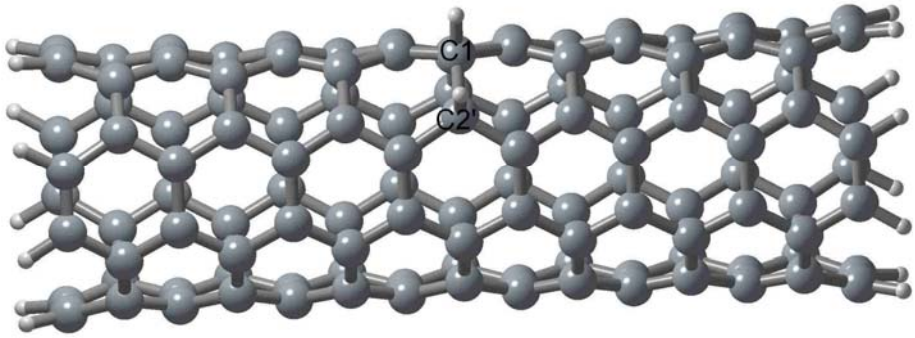

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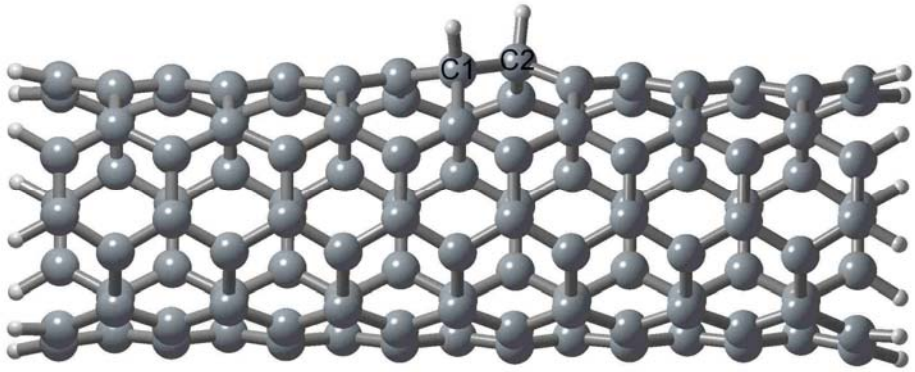

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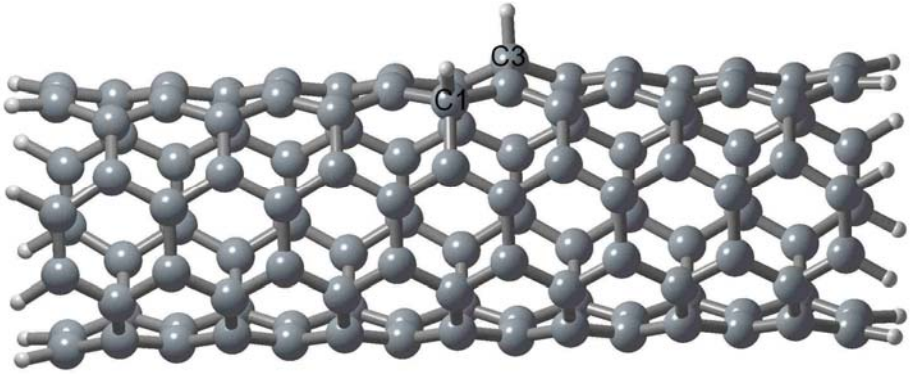

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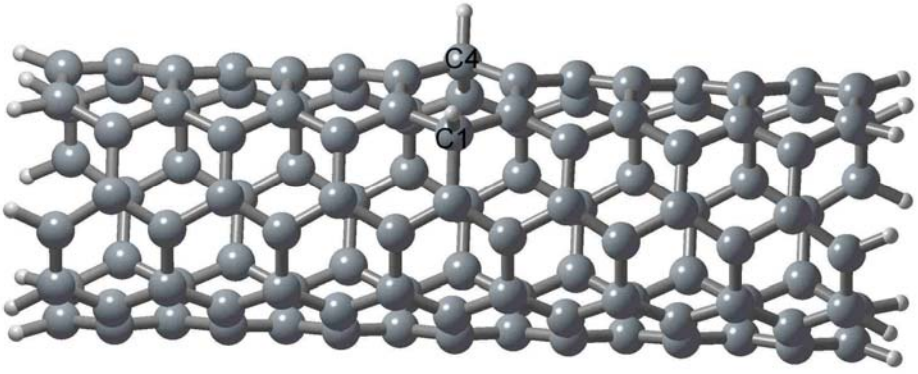

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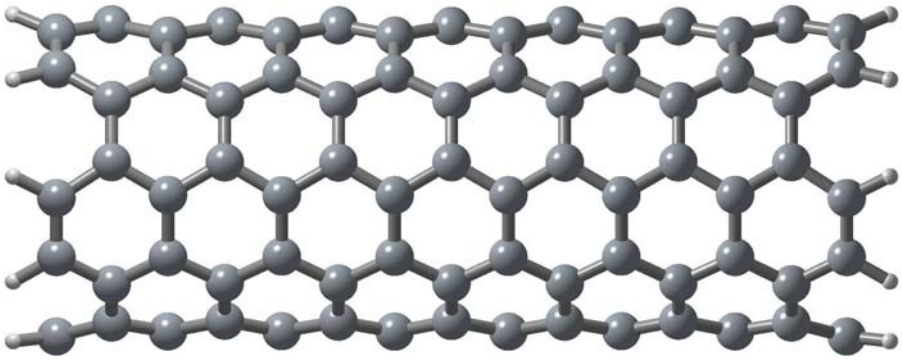

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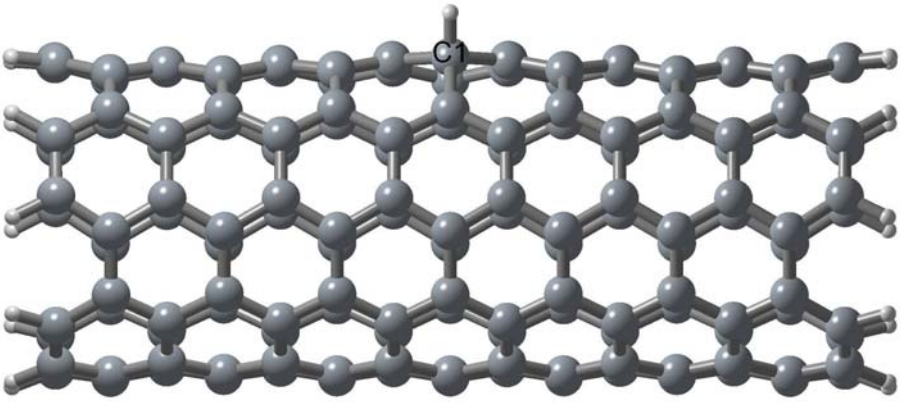

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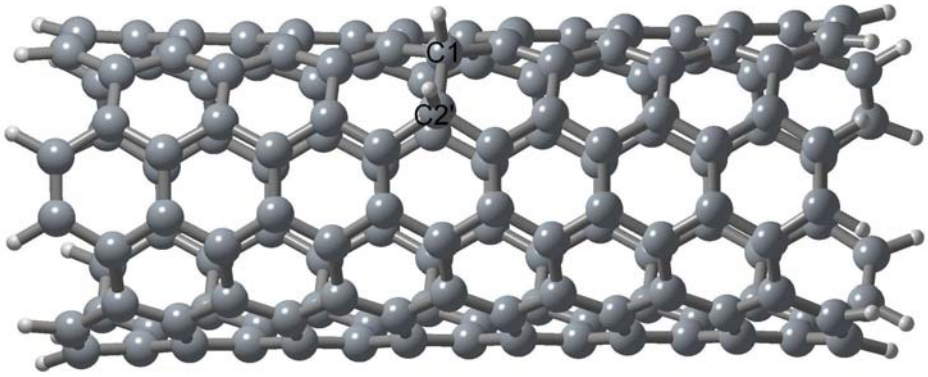

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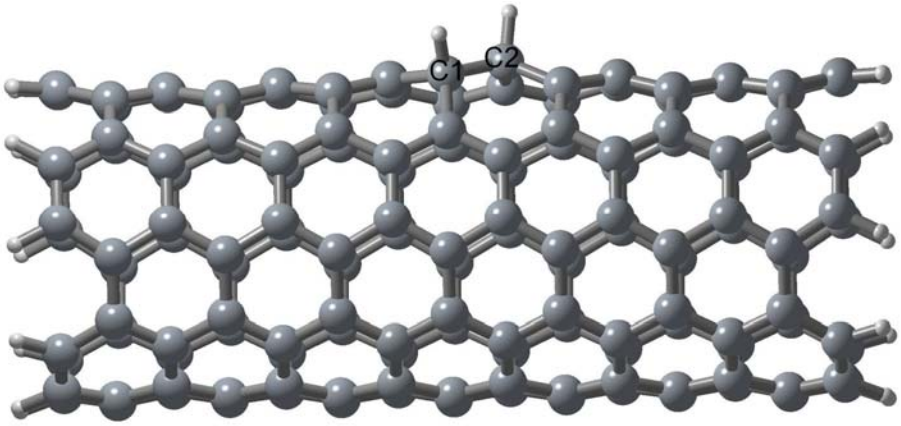

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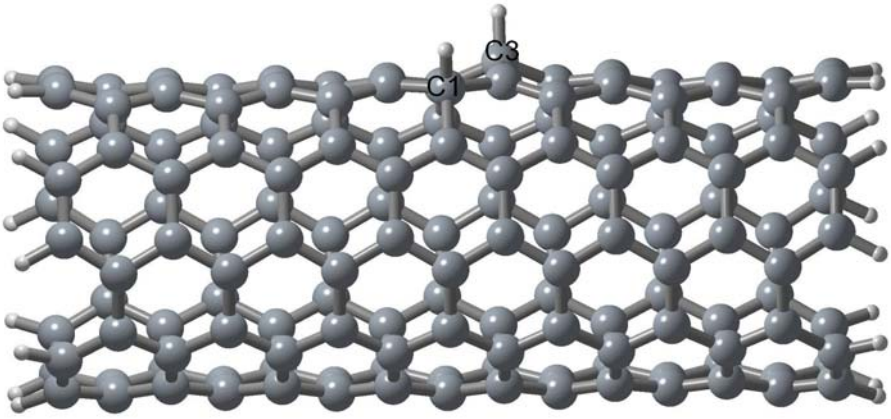

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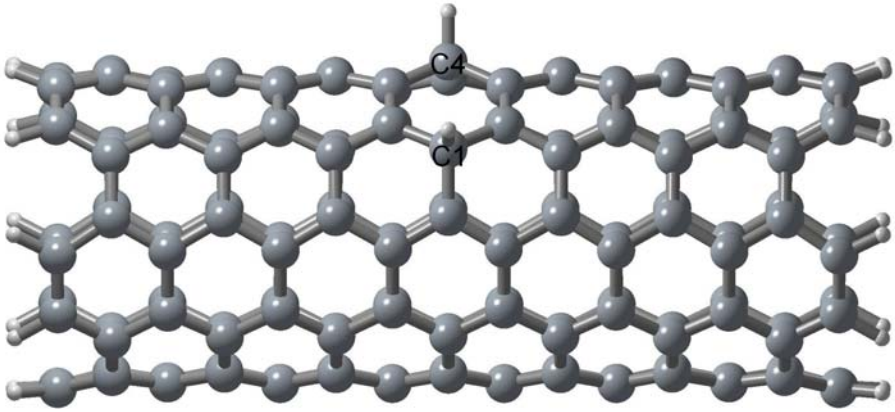

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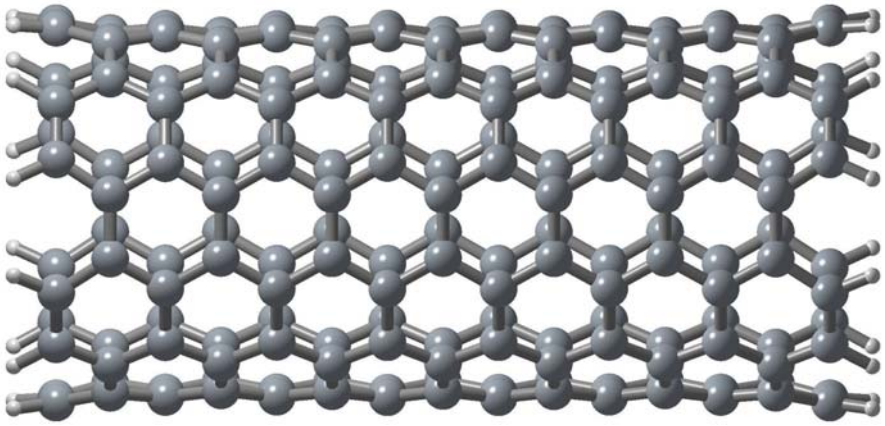

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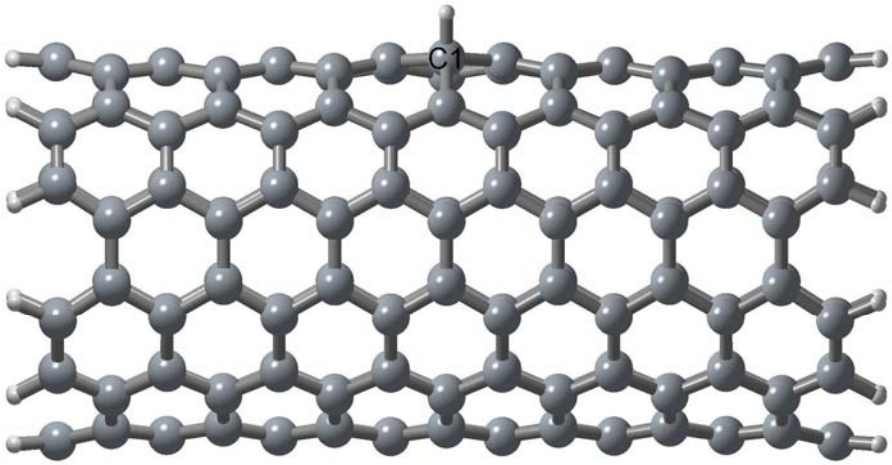

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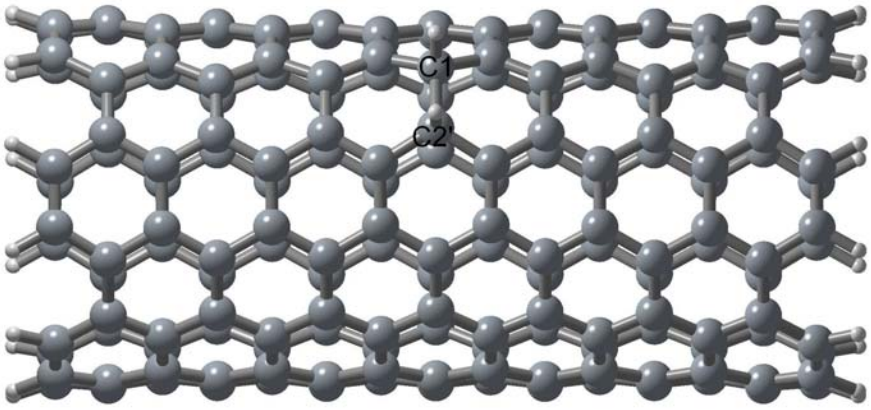

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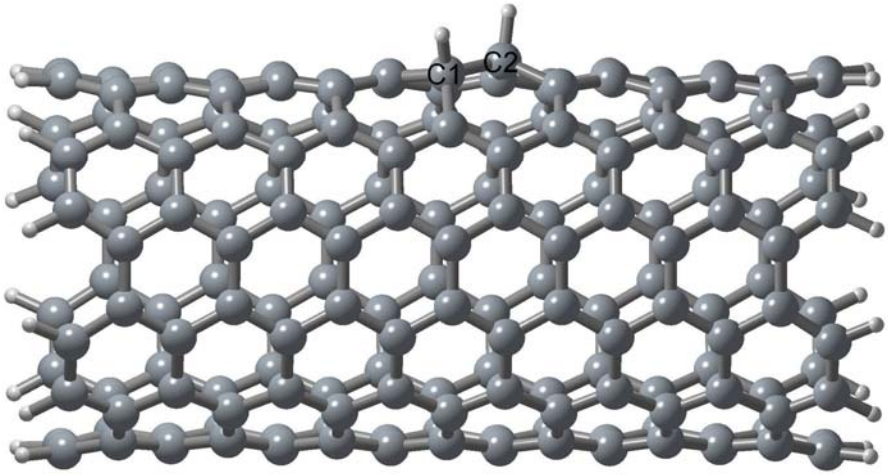

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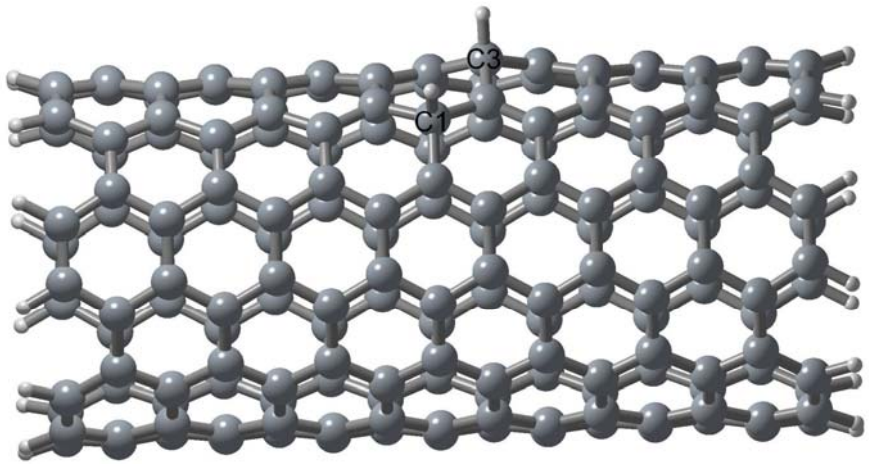

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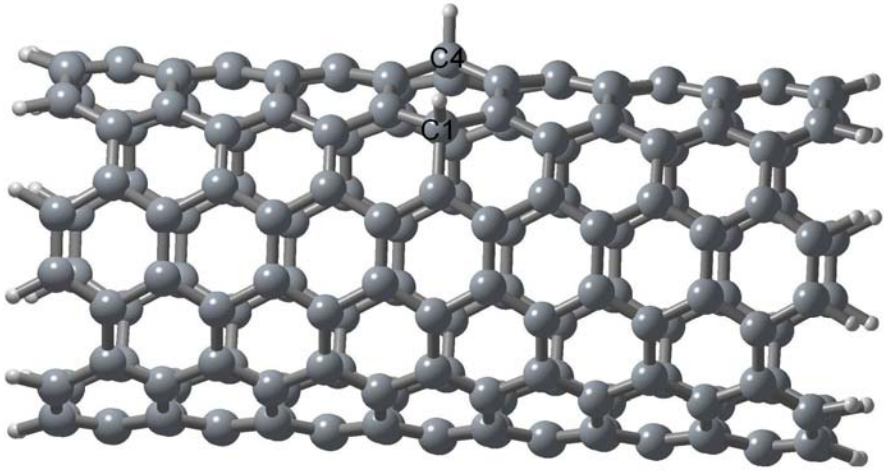

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Figure S3: B3LYP/6-31G(d) optimized geometries of 15 carbon layered nanotubes of (3,3), (4,4), (5,5) and (6,6) armchair SWNTs and their one and two hydrogen chemisorbed structures in horizontal view.